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User's Guide for the Gas Chromatography Automation System

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This document was written as a guide for users of the Advanced GC data system (EPA-600/4-79-038).

The document contains the prescribed procedures for operating the advanced GC system from a user's viewpoint. Also contained in the document is a description of the system manager's duties and responsibilities in maintaining the GC system.

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USER'S GUIDE FOR THE GAS CHROMATOGRAPHY AUTOMATION SYSTEM

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati, conducts research to:

+ Develop and evaluate techniques to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.

+ Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water; and to determine the responses of aquatic organisms to water quality.

+ Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.

+ Develop and operate a computerized system for instrument automation leading to improved data collection, analysis, and quality control.

This report was developed in the Advanced Instrumentation Section of the Environmental Monitoring and Support Laboratory in the interest of advancing laboratory techniques and quality control through computerization.

Dwight G. Ballinger
Director
Environmental Montioring and Support
Laboratory - Cincinnati

ABSTRACT

This document contains a user's guide and a system manager's guide for the Gas Chromatography Automation System of the EPA Laboratory Automation Project.

The Gas Chromatography Automation System accepts reports from a Varian 220L Chromatography Data System, and it uses the data from these reports to perform multi-point calibration, calculation of concentrations, identification of compounds, calculation of relative retention times, and calculation of EPA standard quality control statistics. The system also has the capability to transfer the results to EPA's sample file control system.

This report was submitted in partial fulfillment of Task No. 79-219 by the SouthWestern Ohio Regional Computer Center of the University of Cincinnati. It covers work done between January 10, 1979 and May 4, 1979.

CONTENTS

Foreword.....iii
Abstract.....iv

1. Introduction.....1
2. Using the Varian with this System.....2
3. Signing on to the System.....4
4. General Principles of the System.....6
5. Method Interactions.....8
   - Generating a New Method.....8
   - Modifying a Method.....9
   - Deleting an Existing Method.....10
   - Displaying an Existing Method.....10
6. Concentration Pattern Interactions.....11
   - Creating a New Concentration Pattern.....11
   - Deleting a Concentration Pattern.....11
   - Displaying a Concentration Pattern.....11
   - Listing the Concentration Patterns.....11
7. Calibration.....13
8. Calibration Curve Plotting.....17
9. Injection Listing.....19
10. Processing.....21
11. Quality Control.....23
    - Control Standards.....23
    - Spiked Samples.....23
    - Duplicate Samples.....24
    - Surrogate Spikes.....24
12. Replicate Statistics.....26
13. Dissimilar Analysis Confirmation.....27
14. Sample File Control.....28

Appendices

A. Commonly Used CAS Registry Numbers.....30
B. Notes to the System Manager.....35

SECTION 1

INTRODUCTION

The Gas Chromatography Automation System (GCAS) is an elaborate extension of the Varian 220L Chromatography Data System. In this arrangement, you will use the Varian to control your instrument and to collect data. The data will be automatically transferred to the GCAS, and you will be able to perform several types of multi-point calibrations, plot your calibration curves, calculate concentrations, perform EPA standard quality control calculations, calculate replicate statistics, perform dissimilar analysis confirmations, and report your results to the Sample File Control System.

The GCAS is designed to be as self-explanatory and mistake-proof as possible. The questions it asks are clear and complete. If you give an unreasonable answer to a question, the GCAS will tell you so, and it will ask you the same question again. Furthermore, no matter what mistake you may make, the GCAS will not allow you to destroy any data that it received from the Varian. Therefore, if you make a serious mistake, you can always start over with no harm done. Feel free to experiment with the GCAS.

SECTION 2

USING THE VARIAN WITH THIS SYSTEM

It is never necessary to work with both the Varian and the GCAS at the same time. Rather, you will operate the Varian according to its normal procedures and then use the GCAS for processing the data which the Varian has collected. There are, however, a few points to keep in mind while you are using the Varian.

First, your Varian method number will also be your method number in the GCAS. You will have to cooperate with other users so that you will not try to use someone else's method number. The computers cannot enforce this cooperation.

When you create a method in the Varian, you have to provide an identifier for each compound or group of co-eluting compounds. The GCAS will not accept any identifier containing a comma. An identifier may be any series of up to eight characters or spaces, but since the identifiers will be used throughout the GCAS, you will want to pick memorable ones. For example, your identifier for bromoform might be "CHBR3" or perhaps "BROMFORM." There will not be any problem if two methods happen to use the same identifier for different compounds, nor if two methods happen to have different identifiers for the same compound. The only restrictions are that within a single method, every identifier must be unique, and that in different methods which are to be used for dissimilar analysis confirmation, the identifiers of interest must be exactly the same.

The title which you give to a Varian report will be carried into the GCAS for your reference. The only restrictions on specifying a title are that the title cannot consist of more than thirty characters and spaces, and it cannot contain a comma. Typical titles might be "THIRD STANDARD - 20UG/L EACH" or "SAMPLE 46 SPIKED 10UG/L EACH."

The transfer of data from the Varian to the GCAS is done automatically by a special microcomputer. All you need to do is specify that your reports be printed on your own Varian terminal and one of the Varian terminals which have been connected to the microcomputer. Ask the Varian system manager which terminal(s) you should specify.

When your Varian report reaches the GCAS, it will be assigned an injection ID number which you will need to know in order to use the data. Since the injection ID numbering scheme is easily predictable, you will be able to write down the ID number for each injection without having to sign on to the GCAS. Injection ID numbers are of the form "IIMMDDSS", where "II" is your

Varian instrument number, "MM" is the month, "DD" is the day of the month, and "SS" is the sequence number for the particular instrument that day. For example, the sixth injection into instrument number nine on April 23, would be assigned injection ID number "09042306."

The GCAS automatically keeps track of the sequence number portion of injection ID numbers, and it sets the sequence number for an instrument back to "01" whenever the date of an injection is different from the date of the previous injection into the same instrument. However, if you have a set of injections which will take more than one calendar day to complete, and if you want their sequence numbers to be one long series, you can prevent the GCAS from changing the date in the ID numbers. This ability may be particularly useful to you if you have an autoinjector running unattended past midnight. Simply put "DATEMMDD" in the "operator identification" field of your Varian reports, where "MM" is the month, and "DD" is the day of the month. For example, to freeze the date at April 23, you would put "DATE0423" in the operator identification field. When you use this feature, the GCAS will use the date you specify, and the sequence numbers will continue to accumulate until you change the specified date. Obviously, it is important to change that date before the sequence number reaches 100. This entire feature is optional. If you do not want to use it, leave the operator identification field blank (or use it for your own purposes, but do not put the word "DATE" in it).

The GCAS will store data for at most 100 injections for each instrument. When you have reached the limit of 100 extant injection ID numbers for your instrument, the oldest injection data will be displaced by new data on a "first in/first out" basis.

SECTION 3

SIGNING ON TO THE SYSTEM

The Gas Chromatography Automation System is a set of twenty-two BASIC programs which run in a Nova 840 minicomputer. To use the GCAS, you must first sign on to the Nova. Make sure that you use a terminal which is connected to the Nova and set for full duplex, no parity, and 300 baud (or 1200 baud, if allowed by the Nova system manager).

To get the attention of the Nova, press the ESCAPE key once. (Some Tektronix terminals do not have an ESCAPE key. On such terminals, hold down the CONTROL and SHIFT keys, and press the K key.) If the Nova system is already servicing as many users as it can, it will respond with "ALL LINES BUSY," but normally it will ask for your "ACCOUNT ID." Type the four-character account ID that was assigned to you by the Nova system manager. The four letters will not appear on your terminal as you type them.

Next, the Nova system will usually print some message of the day, and then it will automatically transfer control to the GCAS. This protects the integrity of the GCAS by making it impossible for any user to change the programs or data files. If you want to write your own BASIC programs, you will need to sign on to the Nova under a different account ID.

The GCAS will immediately ask you "WHICH MASTER OPTION DO YOU WANT TO USE? (0-10, OR 'RETURN' FOR HELP)". If you press the return key, the GCAS will print a list of the master options and then ask you the question again, as shown in Figure 1. If you select option 0 (zero, not the letter O), the GCAS will automatically sign you off from the Nova.

```
THESE ARE THE MASTER OPTIONS:

     0.  SIGN OFF
     1.  METHOD INTERACTION
     2.  CONCENTRATION PATTERN INTERACTION
     3.  CALIBRATION
     4.  CALIBRATION CURVE PLOTTING
     5.  INJECTION LISTING
     6.  PROCESSING
     7.  QUALITY CONTROL
     8.  REPLICATE STATISTICS
     9.  DISSIMILAR ANALYSIS CONFIRMATION
    10.  SAMPLE FILE CONTROL

WHICH MASTER OPTION DO YOU WANT TO USE?  (0-10, OR 'RETURN' FOR HELP)
```

Figure 1. The master options question.

SECTION 4

GENERAL PRINCIPLES OF THE SYSTEM

There are several general principles for using the GCAS which apply to all of its options. The first of these is that any time you answer a question, you must follow your answer with a RETURN. If the GCAS asks you to type a number, and you type a character that is not a number, the bell in your terminal will ring, and a question mark will be printed. If this happens, simply type the correct answer, and the GCAS will proceed.

If you make a typing error and notice it before you press RETURN, you can correct it. Pressing the RUBOUT key (the DELETE key on some terminals) will eliminate the last character typed. Typing a backslash (\) will eliminate your entire entry.

Whenever you complete an option in the GCAS, you will be returned to the question, "WHICH MASTER OPTION DO YOU WANT TO USE? (0-10, OR 'RETURN' FOR HELP)". Furthermore, at any point in the GCAS, if you press the ESCAPE key (or the Tektronix CONTROL, SHIFT K), you will also be returned to this master options question. You can use this escape feature to get out of a situation where you have made a mistake or simply to cut short any process. Pressing ESCAPE will not get you out of the GCAS. The only way to get out of the GCAS is to select master option 0.

The first time in a session that you choose a master option other than interacting with a method or performing a dissimilar analysis confirmation, the GCAS will ask you for the number of the method you want to use. It will continue to use the same method for the rest of the session, or until you interact with a method or perform a dissimilar analysis confirmation. After either of these two options, the GCAS will once again ask for your method number.

It is never appropriate to type a comma in the GCAS. For example, to enter the number one million, you must type "1000000". If you are typing the name of a chemical compound which must have a comma in it, type a slash (/) where you want a comma to appear. For example, you might type "1/2/3-TRIMETHYLBENZENE", and the GCAS would change it to "1,2,3-TRIMETHYLBENZENE". This cumbersome arrangement is necessary due to a limitation of the BASIC language in the Nova. The slash technique has been implemented only for the names of compounds.

When the GCAS asks you a question that can be answered by "Y" or "N" (that is, yes or no), just pressing RETURN is the same as answering "N".

At many points in the GCAS, the Nova will do thousands of operations for every one that you do, while at the same time it is also servicing several other users. Consequently, slight delays are perfectly normal. If the GCAS appears to have stalled, wait at least two minutes before you give up and press ESCAPE.

There is no limit to the number of people who can use the GCAS at one time, as long as they all use their own data. No two people can ever use the same method or injection data at the same time.

If you find any error in the GCAS, make a detailed record of what lead up to it. Bring this to the attention of the Advanced Instrumentation Section, and the problem will be corrected.

SECTION 5

METHOD INTERACTIONS

To interact with a method, you must select master option 1. There are four types of method interactions: 1) generate a new method, 2) modify an existing method, 3) delete an existing method, and 4) display an existing method.

GENERATING A NEW METHOD

To create a new method, the GCAS will ask you to type a lot of information, but once you have established the method, you can use it indefinitely. When the GCAS asks, "WHAT SHOULD BE THE NUMBER FOR THE NEW METHOD?" you will probably want to use your Varian method number to avoid confusion, but you may use any number between 1 and 9999 inclusive, as long as the number is not already assigned to a different GCAS method.

You will next have to select the type of method. The choices are: 1) internal standards (not implemented in Version I of the GCAS), 2) purge and trap with external standards, 3) liquid/liquid extraction with external standards, and 4) direct aqueous injection with external standards. Your choice of method type will influence how the GCAS performs calibration and concentration calculations.

Next, you must select the type of retention time calculations from either 1) relative retention times, or 2) capacity ratios. If you select relative retention times, you will also have to enter the identifier for the compound to whose retention time all others are relative. Then during processing, relative retention times for all of the peaks will be calculated by the formula:

$$\text{Rel. Retn. Time} = \frac{\text{Retn. Time}}{\text{Retn. Time of Reference}} \times 100.$$

If you choose capacity ratios instead of relative retention times, you will have to enter your dead volume time in seconds. Then during processing, capacity ratios for all peaks will be calculated by the formula:

$$\text{Capacity Ratio} = \frac{\text{Retn. Time}}{\text{Dead Volume Time}} - 1.$$

When you type the identifiers for the method, be sure to spell them exactly the same way you did in the Varian. The identifiers do not have to be in any particular order. When the GCAS asks "NUMBER OF COMPOUNDS? (1, 2, OR 3)" enter the number of co-eluting compounds which are associated with the identifier. The names of compounds may contain up to forty characters.

The Chemical Abstracts Services (CAS) Registry numbers are required by the GCAS only if you intend to send your results to the Sample File Control System. If you do not need to use CAS numbers, simply press RETURN when the GCAS asks "CAS NUMBER?" If you do type a CAS number, the GCAS will check it for typing errors, but the GCAS cannot check whether you have typed the correct CAS number for the compound named.

When you have entered all of the identifiers for your method, type the word "END" as the next identifier. A method may not contain more than sixty identifiers.

MODIFYING A METHOD

There are four types of method modification: 1) add an identifier, 2) delete an identifier, 3) add another co-eluting compound to the list for an identifier, and 4) change retention time data. If none of these features will change what you need to change, you can delete the troublesome identifier and then put it back in correctly as a new identifier, or you can delete the entire method and start over.

Adding an Identifier

Adding extra identifiers is just like entering the identifiers when you originally create a method. You may add as many as you need up to a total of sixty. Type the word "END" as an identifier when you do not want to add any more. When you add an identifier to a method, the GCAS will delete all of the concentration patterns for that method, since they would no longer be complete.

Deleting an Identifier

To delete an identifier for a method, you simply have to type it correctly, and the GCAS will confirm that it has been deleted.

Adding Another Co-eluting Compound

If you discover that another compound is co-eluting with one of your named compounds, you can add the name and CAS number of the additional compound to the list of compounds associated with the established identifier. No identifier can have more than three co-eluting compounds associated with it.

Changing Retention Time Data

If you use this feature, you will be able to answer the retention time questions from the method generation process again, without deleting the method.

DELETING AN EXISTING METHOD

To delete a method, you only need to type the method number, and the GCAS will confirm that the method has been deleted. All of the concentration patterns associated with a method will automatically be deleted also.

DISPLAYING AN EXISTING METHOD

To display a method, you must type the method number. Then the GCAS will print a method report, as shown in Figure 2.

M-E-T-H-O-D R-E-P-O-R-T

ANALYST: JOHN DOE METHOD NUMBER: 8001
TYPE OF METHOD: PURGE AND TRAP
IDENTIFIER FOR RELATIVE RETENTION TIME REFERENCE PEAK: CHCL3

	IDENTIFIER	NAME OF COMPOUND	CAS NUMBER
1.	CHCL3	CHLOROFORM	67-66-3
2.	CHBRCL2	BROMODICHLOROMETHANE	75-27-4
3.	CHBR2CL	DIBROMOCHLOROMETHANE	124-48-1
4.	CHBR3	BROMOFORM	75-25-2

Figure 2. Typical method report.

SECTION 6

CONCENTRATION PATTERN INTERACTIONS

A concentration pattern is a list of concentrations for the identifiers in your method. Concentration patterns are used as the prepared concentrations of calibration standards and control standards and as the added concentrations for spiked samples. There are four types of concentration pattern interaction: 1) create a new concentration pattern, 2) delete an existing pattern, 3) display an existing pattern, and 4) list the names of the concentration patterns for your method.

CREATING A NEW CONCENTRATION PATTERN

To create a concentration pattern, you must first answer the question "WHAT SHOULD BE THE LETTER NAME FOR THE NEW PATTERN? (A, B, C, ..., OR Z)". You may use any letter of the alphabet for the name of a concentration pattern, as long as the letter is not already assigned to an existing pattern for your method. You will next need to choose the unit of concentration from either 1) nanograms per microliter, or 2) micrograms per liter. Then you will be asked to type the concentrations of all of the identifiers in your method. You will need to create one concentration pattern for each calibration standard, control standard, and spike that you intend to use.

DELETING A CONCENTRATION PATTERN

To delete a concentration pattern, you must simply type the letter name of the pattern, and the GCAS will confirm that the pattern has been deleted.

DISPLAYING A CONCENTRATION PATTERN

To display the contents of a concentration pattern, you must type the letter name of the pattern, and the GCAS will print a concentration pattern report, as shown in Figure 3.

LISTING THE CONCENTRATION PATTERNS

To have the GCAS print a list of concentration patterns for your method, you do not need to do anything other than select this feature. A sample concentration pattern list is shown in Figure 4.

C-O-N-C-E-N-T-R-A-T-I-O-N P-A-T-T-E-R-N R-E-P-O-R-T

CONCENTRATION PATTERN: G METHOD NUMBER: 0200

IDENTIFIER	CONCENTRATION
BZ	80.000
TOLU	80.000
ETBZ	80.000
P XYL	80.000
M XYL	80.000
O XYL	80.000
IPBZ	80.000
STYRENE	80.000
NPBZ	80.000
T BBZ	80.000
SEC BBZ	80.000
124TMBZ	80.000
N BBZ	80.000
BZFURAN	80.000

Figure 3. Typical concentration pattern report.

C-O-N-C-E-N-T-R-A-T-I-O-N P-A-T-T-E-R-N L-I-S-T

CONCENTRATION PATTERNS FOR METHOD 0200: A, B, C, D, E, F, G, H, I, J

Figure 4. Typical concentration pattern list.

SECTION 7

CALIBRATION

When you choose master option 3, the GCAS will begin a calibration procedure. In Version I of the GCAS, there are two calibration procedures, one for external standards calibration using purge and trap processing, and the other for external standards calibration using either liquid/liquid extraction or direct aqueous injection. The GCAS will automatically use the correct calibration procedure for your method, based on an answer you gave to a question during method generation. The two calibration procedures will be discussed together here since there is only one noticeable difference between them.

As calibration begins, the GCAS asks "DO YOU WANT TO CALIBRATE ALL IDENTIFIERS OF METHOD XXXX AT ONCE? (Y OR N)". If you answer "N", the GCAS will ask, "DO YOU WANT TO CALIBRATE XXXXXXXX? (Y OR N)" for each identifier of your method. This allows you to calibrate all of your identifiers at once, and, in a second session, to recalibrate individual identifiers to discard outliers.

The GCAS will then ask for the injection ID numbers for your calibration standards, the concentrations patterns for your standards, and (for liquid/liquid extraction and direct aqueous injection) the injection volumes in microliters. Type "END" as an injection ID when you do not want to enter any more standards information. The GCAS will accept up to 15 calibration standards, including any replicates.

The GCAS will then give you the choice of four types of curve fitting: 1) linear regression, 2) quadratic regression, 3) linear interpolation extended to the origin, and 4) linear regression forced through the origin. Linear regression will find the equation of the straight line which most nearly passes through all of your calibration points. The equation of the line will be of the form

$$C = sA + t$$

where C is the concentration and A is peak area. You must use at least three standards to perform linear regression, because fewer standards would not be enough to prove that the response from your detector is linear. An example of a linear regression is shown in Figure 5.

Quadratic regression will find the equation of the parabola which most nearly passes through the calibration points and which is of the form

$$C = rA^2 + sA + t.$$

You must use at least four standards for this type of fit, because fewer standards would not be enough to prove that the response from your detector is parabolic. An example of a quadratic fit is shown in Figure 6.

Linear interpolation simply connects the calibration points with line segments. A segment is also produced from the origin to the lowest standard. Linear interpolation can be done with one or more standards. Figure 7 shows a linear interpolation.

Linear regression forced through the origin finds the equation of the line which passes through the origin and most nearly passes through all of the calibration points. The equation is of the form

$$C = sA.$$

At least three standards are required for this type of fit. An example of a forced-origin regression is shown in Figure 8.

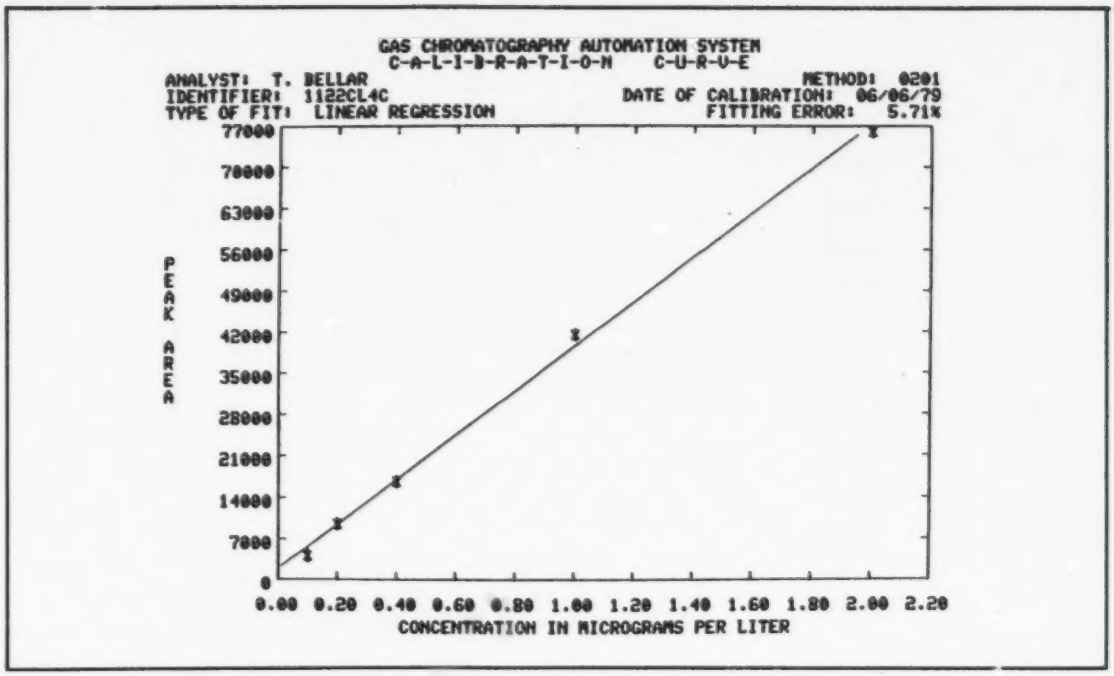

Figure 5. Typical linear regression calibration curve.

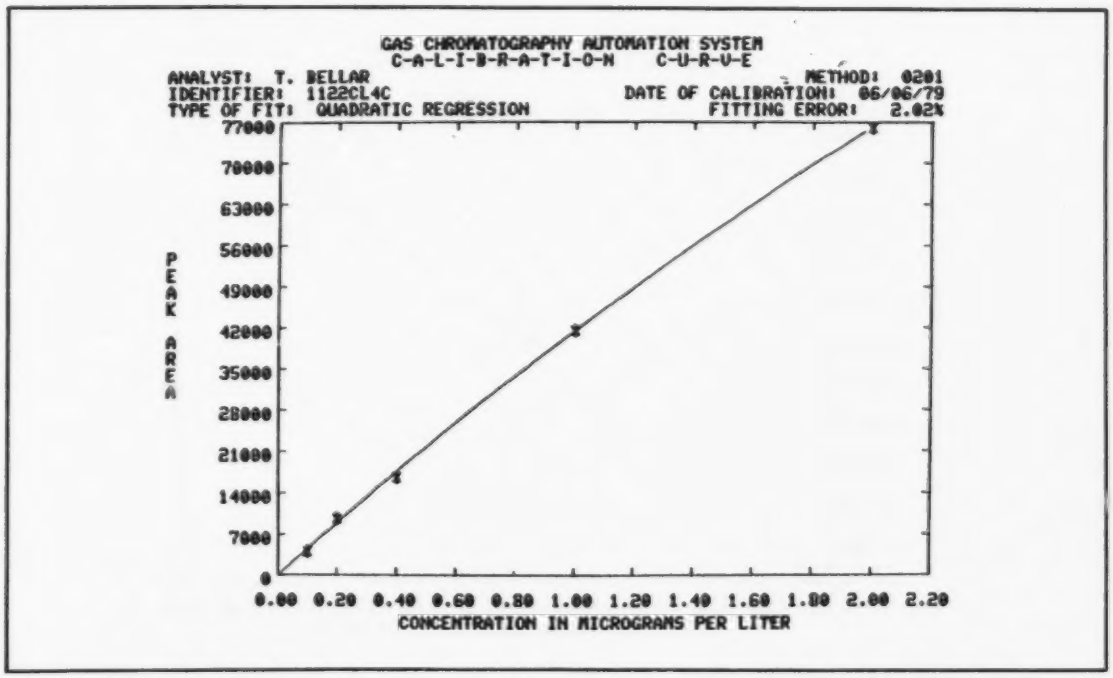

Figure 6. Typical quadratic regression calibration curve.

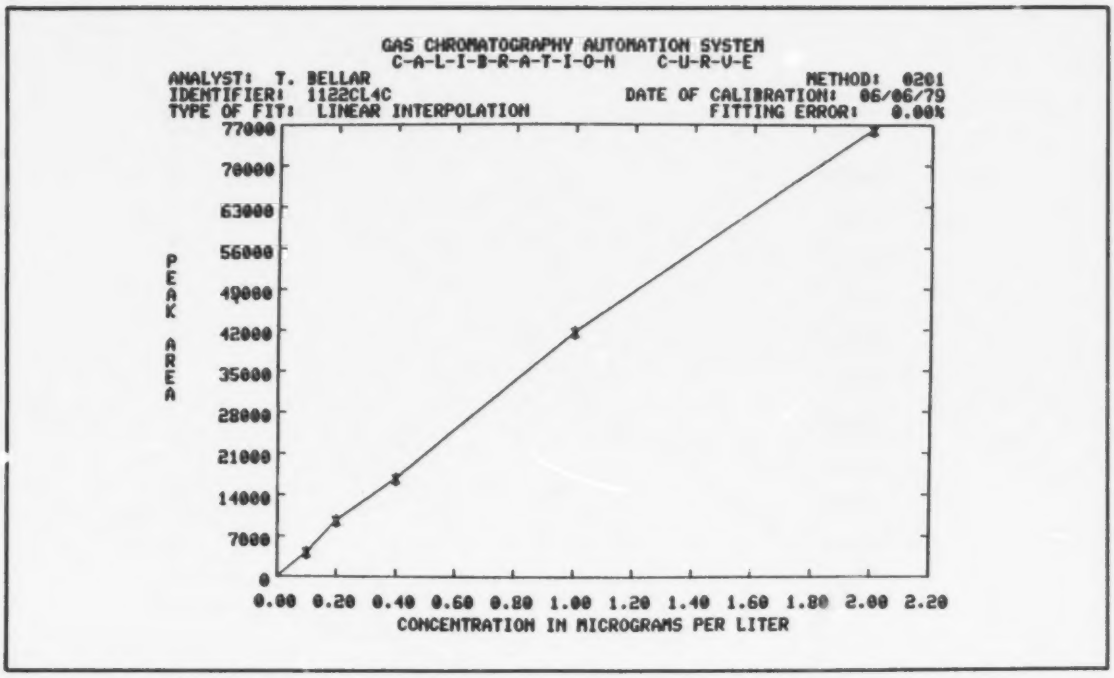

Figure 7. Typical linear interpolation calibration curve.

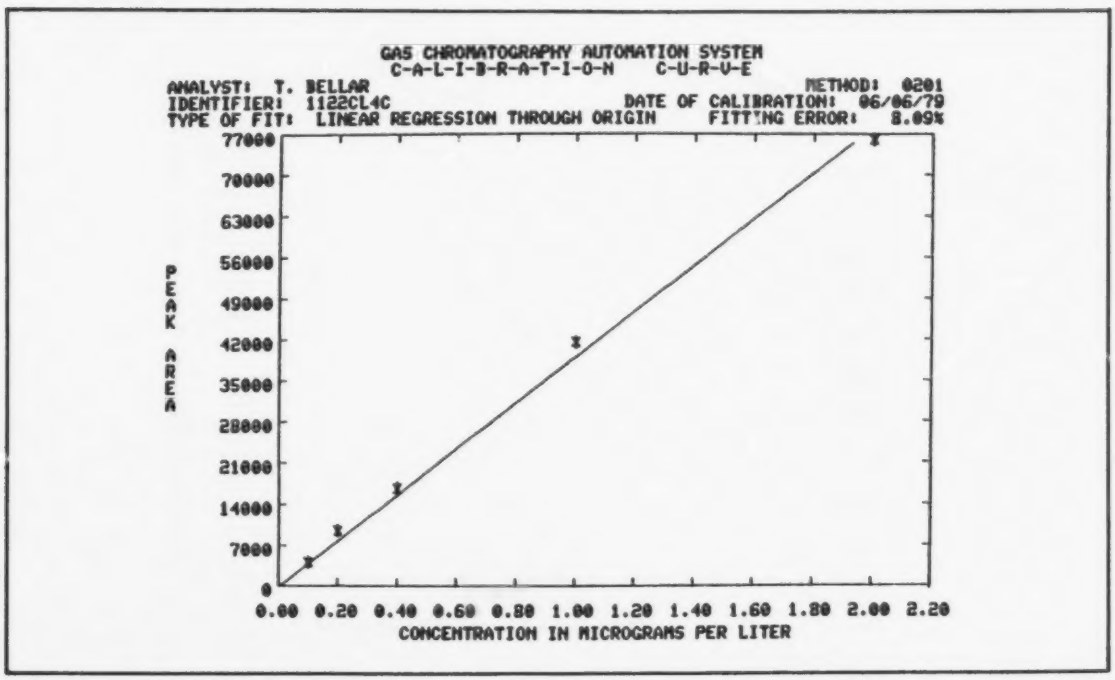

Figure 8. Typical forced origin calibration curve.

SECTION 8

CALIBRATION CURVE PLOTTING

Calibration curve plotting can be done by selecting master option 4. The GCAS must first ask you what type of terminal you are using, since the plotting feature of this option was designed specially for either Tektronix 4000 Series terminals or Hewlett-Packard 2647 or 2648 terminals. However, if you are not using one of these specific terminals, you can still get useful information from this option.

After you have typed the identifier for which you want a calibration curve plot, the GCAS will clear the screen and draw the picture, as shown in Figures 5, 6, 7, and 8. When the picture is complete, the bell in your terminal will be sounded five times to inform you that you may make a hard copy. When you are ready to proceed, press RETURN, and the GCAS will clear the screen and print a table of residuals as shown in Figure 9. If you are not using a plotting terminal, the plotting feature will be skipped, but the data shown in Figure 9 will be printed.

The GCAS provides a "fitting error" statistic to help you judge your calibration curves. The fitting error is actually a percent, relative, standard error of estimate (also known as the coefficient of variation). It is calculated by the formula:

$$\frac{\sqrt{\frac{\Sigma\,(\text{Known Conc.} - \text{Calculated Conc.})^2}{\text{Number of Standards} - 2}}}{\text{Mean Conc.}} \times 100.$$

A fitting error of 0.0% indicates a perfect fit; that is, the curve passes through all of the calibration points. Other fitting error values are meaningful only in terms of comparison and experience. For example, in Figures 5, 6, 7, and 8, the same points have been fit four different ways. The fitting errors can be used comparatively to prove that linear regression (5.71% fitting error) is a better fit than linear regression forced through the origin (8.09% fitting error) but not as good as quadratic regression (2.02% fitting error) for these specific points. Furthermore, experience has shown that any curve having a fitting error greater than about 5.0% is not good enough to use. Some analysts have been able to routinely get fitting errors of about 2.0%.

Fitting errors cannot be used to judge linear interpolation, since by definition interpolation always produces a fitting error of 0.0%, no matter how poor the curve is.

C-A-L-I-B-R-A-T-I-O-N D-A-T-A R-E-P-O-R-T

ANALYST: T. BELLAR METHOD: 0201

IDENTIFIER: 1122CL4C DATE OF CALIBRATION: 04/30/79

TYPE OF FIT: LINEAR REGRESSION THROUGH ORIGIN FITTING ERROR: 8.09%

INJECTION ID	PEAK AREA	PREPARED	CALCULATED	DIFFERENCE
01030101	76236	2.000	1.949	+0.051
01030102	41738	1.000	1.067	-0.067
01030103	16905	0.400	0.432	-0.032
01030104	9779	0.200	0.250	-0.050
01030105	4327	0.100	0.111	-0.011

EQUATION: CONCENTRATION = +2.56E-05(A)

Figure 9. Typical calibration data report.

SECTION 9

INJECTION LISTING

If you get confused about your injection ID numbers, you can use master option 5 to find out what ID number has been assigned to each injection. There are three types of reports which this option can generate: 1) all extant injection ID numbers from one instrument, 2) ID numbers for a specific date from one instrument, and 3) the title of the Varian report for any ID number from any instrument.

To get the first type of report, you only need to type your Varian instrument number, and the GCAS will print a report such as that shown in Figure 10. The injection ID numbers on this report are in reverse chronological order.

E-X-T-A-N-T I-N-J-E-C-T-I-O-N-S R-E-P-O-R-T

INSTRUMENT NUMBER: 02 ALL INJECTIONS

02060409	02060408	02060407	02060406	02060405	02060404
02060403	02060402	02060401	02060103	02060102	02060101
02053002	02053001	02052502	02052501	02052408	02052407
02052406	02052405	02052404	02052403	02052402	02052401
02052301	02052205	02052204	02052203	02052202	02052201
02052103	02052102	02052101	02050301	02050213	02050212
02050211	02050210	02050209	02050208	02050207	02050206
02050205	02050204	02050203	02050202	02050201	02050114
02050113	02050112	02050111	02050110	02050109	02050108
02050107	02050106	02050105	02050104	02050103	02050102
02050101	02043013	02043012	02043011	02043010	02043009
02043008	02043007	02043006	02043005	02043004	02043003
02043002	02043001	02042710	02042709	02042708	02042707
02042706	02042705	02042704	02042703	02042702	02042701
02042313	02042312	02042311	02042310	02042309	02042308
02042307	02042306	02042305	02042304	02042303	02042302
02042301	02042014	02042013	02042012		

Figure 10. Typical extant injections report.

To get the second type of report, you need to also specify the month and day of interest. The GCAS will produce a report similar to that shown in Figure 11.

Figure 12 shows how to get the title of the Varian report associated with an injection ID number. Figure 12 also shows the type of messages which the GCAS will print if you try to use an injection whose Varian report was faulty.

```
                E-X-T-A-N-T   I-N-J-E-C-T-I-O-N-S   R-E-P-O-R-T
INSTRUMENT NUMBER:  02                MONTH:  06                DAY:  04

02060409     02060408     02060407     02060406     02060405     02060404
02060403     02060402     02060401
```

Figure 11. Typical extant injections report for one day.

```
WHAT ID?  02050102

FOR ID 02050102, THE REPORT TITLE IS '20/500 STD #10.'

DO YOU WANT TO PRINT THE TITLE FOR ANOTHER ID?  (Y OR N)  Y

WHAT ID?  01021902

01021902 CANNOT BE USED BECAUSE THE REPORT DID NOT HAVE A TOTAL AREA.

DO YOU WANT TO PRINT THE TITLE FOR ANOTHER ID?  (Y OR N)  Y

WHAT ID?  01022301

01022301 CANNOT BE USED BECAUSE THE REPORT WAS IN THE WRONG FORMAT.

DO YOU WANT TO PRINT THE TITLE FOR ANOTHER ID?  (Y OR N)  N
```

Figure 12. Typical reports of injection titles.

SECTION 10

PROCESSING

Processing an injection involves calculating the concentration of every identifier, calculating the relative retention time or capacity ratio for every peak, looking up the full chemical name(s) and CAS Registry number(s) for the identifiers that appear in the Varian report, and printing an injection data processing report. Also, if there is any identifier in your method which is not detected in the injection, the GCAS will add that identifier to the data for the injection with a notation of "NOT DETECTED". Injections must be processed before they can be used for quality control calculations, replicate statistics, or dissimilar analysis confirmation.

In Version I of the GCAS, there are three types of concentration calculations corresponding to three types of sample preparation: 1) purge and trap, 2) liquid/liquid extraction, and 3) direct aqueous injection. The GCAS will automatically use the correct algorithm, based on an answer you gave to a question during method generation.

To initiate the processing routine you must choose master option 6. The GCAS will always ask for the ID number of the injection to be processed. If you are using direct aqueous injection, the GCAS will also ask for the volume of the injection in microliters, and if you are using liquid/liquid extraction, the GCAS will also ask for the volume of the extract in milliliters and the volume of the water extracted in liters.

The rest of the processing procedure is entirely automatic, although somewhat time-consuming. A sample injection data processing report is shown in Figure 13.

GAS CHROMATOGRAPHY AUTOMATION SYSTEM

I-N-J-E-C-T-I-O-N D-A-T-A P-R-O-C-E-S-S-I-N-G R-E-P-O-R-T

ANALYST: JOHN DOE
METHOD NUMBER: 8001
METHOD TYPE: PURGE AND TRAP

INJECTION ID NUMBER: 13060603
REPORT TITLE: SAMPLE NO. 65487245
DATE: 6/ 6/79

	COMPOUND(S)	C.A.S. NUMBER	PEAK TYPE	RETENTION TIME	RELATIVE RETENTION TIME	AREA OF PEAK	CONCENTRATION IN MICROGRAMS/LITER
1.	UNEXPLAINED PEAK			132	78.11	970.0	
2.	UNEXPLAINED PEAK			154	91.12	1011.0	
3.	CHLOROFORM	67-66-3		169	100.00	5588.0	45.224
4.	BROMODICHLOROMETHANE	75-27-4		180	106.51	6838.0	6.951
5.	DIBROMOCHLOROMETHANE	124-48-1		191	113.02	11426.0	32.852
6.	UNEXPLAINED PEAK			205	121.30	1227.0	
7.	BROMOFORM	75-25-2		225	133.14	3048.0	6.745
8.	UNEXPLAINED PEAK			231	136.69	1225.0	
9.	BROMOCHLOROMETHANE						NOT DETECTED

Figure 13. Typical data processing report.

SECTION 11

QUALITY CONTROL

The GCAS is capable of performing four types of quality control calculations: 1) control (check) standards, 2) spiked samples, 3) duplicate samples, and 4) surrogate spikes. Before you begin to use any quality control feature, you must create the necessary concentration patterns and process the appropriate injections.

CONTROL STANDARDS

To get a control standard report like that shown in Figure 14, you only need to type the injection ID number and the concentration pattern letter for your control standard. The concentration pattern should contain the prepared concentrations for all of the identifiers. The GCAS will allow you to use the same concentration patterns for calibration standards and control standards, or establish different concentration patterns for your control standards. The percent recovery of control standards is calculated by the formula:

$$\text{Percent Recovery} = \frac{\text{Measured Concentration}}{\text{Prepared Concentration}} \times 100.$$

In the GCAS, it is allowable to process an injection, use it as a control standard, decide to recalibrate, and use that same injection as a calibration standard.

SPIKED SAMPLES

To get a spiked sample report like that in Figure 15, you must enter the injection ID number for the unspiked sample, the concentration pattern for the spike added values, and the injection ID number for the spiked sample. The percent recovery of spikes is calculated by the formula:

$$\text{Percent Recovery} = \frac{\text{Final Conc. - Orig. Conc.}}{\text{Added Conc.}} \times 100.$$

DUPLICATE SAMPLES

Figure 16 shows a typical duplicate samples report. To get such a report, you only need to type the injection ID numbers of the two samples.

SURROGATE SPIKES

You must type the ID number for the injection containing a surrogate spike, the identifier for the surrogate spike, and the prepared concentration of the surrogate spike to get a report like that in Figure 17. Obviously, you must have calibrated for the surrogate spike compound to make this feature work. The percent recovery of surrogate spikes is calculated by the formula:

$$\text{Percent Recovery} = \frac{\text{Calculated Conc.}}{\text{Prepared Conc.}} \times 100.$$

C-O-N-T-R-O-L S-T-A-N-D-A-R-D R-E-P-O-R-T

INJECTION ID: 13060511 METHOD NUMBER: 8001

CONCENTRATION PATTERN: C CONCENTRATIONS IN MICROGRAMS/LITER

IDENTIFIER	PREPARED CONCENTRATION	MEASURED CONCENTRATION	PERCENT RECOVERED
CHCL3	60.000	61.888	103.1%
CHBRCL2	60.000	62.089	103.5%
CHBR2CL	60.000	59.903	99.8%
CHBR3	60.000	57.979	96.6%
CH2BRCL	60.000	NOT DETECTED	

Figure 14. Typical control standard report.

S-P-I-K-E-D S-A-M-P-L-E R-E-P-O-R-T

INJECTION ID FOR SPIKE ORIGINAL: 13060521 METHOD NUMBER: 8001
CONCENTRATION PATTERN FOR SPIKE ADDED VALUE: C
INJECTION ID FOR SPIKE FINAL: 13060522
CONCENTRATIONS IN MICROGRAMS/LITER

IDENTIFIER	ORIGINAL CONCENTRATION	ADDED CONCENTRATION	FINAL CONCENTRATION	PERCENT RECOVERED
CHCL3	61.888	60.000	117.913	93.4%
CHBRCL2	62.089	60.000	117.035	91.6%
CHBR2CL	59.903	60.000	115.615	92.9%
CHBR3	57.979	60.000	114.237	93.8%
CH2BRCL	NOT DETECTED	60.000	NOT DETECTED	

Figure 15. Typical spiked sample report.

D-U-P-L-I-C-A-T-E S-A-M-P-L-E-S R-E-P-O-R-T

INJECTION ID FOR FIRST MEMBER: 13060527 METHOD NUMBER: 8001
INJECTION ID FOR SECOND MEMBER: 13060528
CONCENTRATIONS IN MICROGRAMS/LITER

IDENTIFIER	FIRST CONCENTRATION	SECOND CONCENTRATION	ABSOLUTE DIFFERENCE
CHCL3	59.668	61.345	-1.678
CHBRCL2	14.726	13.706	+1.020
CHBR2CL	49.693	52.361	-2.667
CHBR3	8.412	7.722	+0.691
CH2BRCL	NOT DETECTED	NOT DETECTED	

Figure 16. Typical duplicate samples report.

S-U-R-R-O-G-A-T-E S-P-I-K-E R-E-P-O-R-T

INJECTION ID: 13060532 METHOD NUMBER: 8001
PREPARED CONCENTRATION OF BROMOCHLOROMETHANE: 30.000
CALCULATED CONCENTRATION: 28.019
PERCENT RECOVERED: 93.4%
CONCENTRATIONS IN MICROGRAMS/LITER

Figure 17. Typical surrogate spike report.

SECTION 12

REPLICATE STATISTICS

To use the replicate statistics option, you must select master option 8 and type the injection ID numbers for all of your replicate injections. You may enter up to ten replicates. The GCAS will print a report like that shown in Figure 18.

R-E-P-L-I-C-A-T-E S-T-A-T-I-S-T-I-C-S R-E-P-O-R-T

METHOD NUMBER: 8001 CONCENTRATIONS IN MICROGRAMS/LITER

REPLICATE INJECTION ID NUMBERS: 13060536, 13060537, 13060538, 13060539

IDENTIFIER	AVERAGE CONCENTRATION	STANDARD DEVIATION	NUMBER OF REPLICATES
CHCL3	22.138	0.20	4
CHBRCL2	23.923	0.42	4
CHBR2CL	22.055	0.03	4
CHBR3	17.690	0.25	4
CH2BRCL			0

Figure 18. Typical replicate statistics report.

SECTION 13

DISSIMILIAR ANALYSIS CONFIRMATION

Master option 9 will allow you to perform a dissimilar analysis confirmation. The GCAS will handle up to four different methods for this feature. Also, to allow for Florisil Column Adsorption Chromatography techniques, you are allowed to enter the injection ID numbers for up to four injections for each method. Dissimilar analysis confirmation is performed for only one identifier at a time.

After you have typed your method numbers, injection ID numbers, and identifier of interest, the GCAS will print a report as shown in Figure 19.

D-I-S-S-I-M-I-L-A-R A-N-A-L-Y-S-I-S C-O-N-F-I-R-M-A-T-I-O-N
IDENTIFIER: CHBR2CL CONCENTRATIONS IN MICROGRAMS/LITER

METHOD NUMBER	INJECTION ID	CALCULATED CONCENTRATION
8001	13060536	22.044
8001	13060537	22.073
8002	14060502	22.021
8002	14060503	22.081

Figure 19. Typical dissimilar analysis confirmation report.

SECTION 14

SAMPLE FILE CONTROL

The basic plan of Sample File Control (SFC) is that when environmental samples arrive in the laboratory, they will be logged into the SFC computer and assigned SFC sample ID numbers. The computer will provide you with a backlog sheet showing which samples need to be analyzed and what compounds are to be measured. You will use the GCAS to calculate the concentrations of the specified compounds, and then the GCAS will enable you to create a "run results file" which you can send back to SFC. SFC will report the results to the requestor, and will provide you with control charts and a historical record of your work.

To create an SFC run results file, you must use master option 10. Although this option is no more difficult to use than the others, it must be used very carefully since the GCAS cannot prevent you from sending erroneous data to SFC, and since the only way to correct most mistakes is to start over. If you press the ESCAPE key while you are using this option, you will return to the master options questions, and your incomplete run results file will be deleted.

When you begin to use this feature, you will be confronted with three types of SFC interaction: 1) create a new run results file, 2) edit or delete an existing run results file, or 3) send an existing run results file to the SFC computer. To create a run results file, you will have to type the parameter/method code (which can be found on your backlog sheet), the measurement instrument ID, and your three initials. Then you can place laboratory control standards data into the run results file by simply typing the injection ID and concentration pattern letter for each standard. Since laboratory control standards are not environmental samples, they do not have SFC sample ID numbers. The SFC system distinguishes between laboratory control standards and instrument check standards, and it has been decided that for gas chromatography, instrument check standards will not be reported to SFC.

Next, you will be able to report the measured concentrations for the samples on your backlog sheet, along with associated QC results. For each sample, you must type the SFC sample ID from the backlog sheet, the injection ID of the sample, the prepared concentration of any surrogate spike, the injection ID's and concentration pattern letters of any spikes, and the injection ID's of any duplicates.

When you have finished the run results file, the name of that file will be displayed. The name of a run results file is the parameter/method code followed by a letter of the alphabet.

Finally, you will be asked again if you want to create, edit, or send the run results file. You do not have to edit your run results file, but you must send it to SFC. If you choose the editing feature, you will be transferred to the RUNEDIT program of the SFC system. Similarily, if you choose the sending feature, you will be transferred to the SFC program named SEND. In both of these programs, you will need to know the name of your run results file. After either of these two programs, you will be returned to the beginning of the GCAS. Check the SFC user's guide for instructions on how to use RUNEDIT and SEND.

APPENDIX A
COMMONLY USED CAS REGISTRY NUMBERS

TABLE A-1. The Forty-Six Compounds of the Base-Neutral Fraction

Compound Name	CAS Registry Number
1,3-Dichlorobenzene	541-73-1
1,4-Dichlorobenzene	106-46-7
1,2-Dichlorobenzene	95-50-1
Hexachloroethane	67-72-1
Bis(2-Chloroethyl) ether	111-44-4
Bis(2-Chloroisopropyl) ether	39638-32-9
N-nitrosodi-n-propylamine	621-64-7
Isophorone	78-59-1
Nitrobenzene	98-59-1
Hexachlorobutadiene	87-68-3
1,2,4-Trichlorobenzene	129-82-1
Naphthalene	91-10-3
Bis(2-Chloroethoxy)methane	111-91-1
Hexachlorocyclopentadiene	77-47-4
2-Chloronaphthalene	91-58-7
Acenaphthylene	208-96-8
2,6-Dinitrotoluene	606-20-2
Acenaphthene	83-32-9
Dimethylphthalate	131-11-3
Fluorene	86-73-7
4-Chlorophenyl phenyl ether	7005-72-3
2,4-Dinitrotoluene	121-14-2
1,2-Diphenylhydrazine	122-66-7
Diethylphthalate	84-66-2
N-Nitrosodiphenylamine	86-30-6
Hexachlorobenzene	118-74-1
4-Bromophenyl phenyl ether	101-55-3
Phenanthrene	85-01-8
Anthracene	120-12-7
Di-n-butylphthalate	84-74-2
Fluoranthene	106-44-0
Pyrene	129-00-0
Benzidine	98-87-5
Butylbenzylphthalate	85-68-7
Bis(2-ethylhexyl)phthalate	117-81-7
Chrysene	218-01-9

(continued)

TABLE A-1 (continued)

Compound Name	CAS Registry Number
Benzo(a)anthracene	56-55-3
Benzo(b)fluoranthene	205-99-2
Benzo(k)fluoranthene	207-08-9
3,3'-Dichlorobenzidine	91-94-1
Di-n-octylphthalate	117-84-0
Benzo(a)pyrene	50-32-8
Indeno(1,2,3-cd)pyrene	193-39-5
Dibenzo(a,h)anthracene	53-70-3
Benzo(g,h,i)perylene	191-24-2
Nitrosodimethylamine	62-75-9

TABLE A-2. The Twenty-Six Compounds of the Pesticide Fraction

Compound Name	CAS Registry Number
β-endosulfan	33213-65-9
α-Benzenehexachloride	319-84-6
γ-Benzenehexachloride	58-89-9
β-Benzenehexachloride	319-85-7
Aldrin	309-00-2
Heptachlor	76-44-8
Heptachlor epoxide	1024-57-3
δ-endosulfan	959-98-8
Dieldrin	60-57-1
4,4'-DDE	72-55-9
4,4'-DDD	72-54-8
4,4'-DDT	50-29-3
Endrin	72-20-8
Endosulfane sulfate	1031-07-8
δ-Benzenehexachloride	319-86-8
Chlordane	57-74-9
Toxaphene	8001-35-2
Aroclor-1242	53469-21-9
Aroclor-1254	11097-69-1
Aroclor-1221	11104-28-2
Aroclor-1232	11141-16-5
Aroclor-1248	12672-29-6
Aroclor-1260	11096-82-5
Aroclor-1016	12674-11-2
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6
Endrin Aldehyde	--

TABLE A-3. The Thirty Compounds of the Purgeable Fraction and Two Direct Aqueous Analytes

Compound Name	CAS Registry Number
Acrolein	107-02-8
Acrylonitrile	107-13-1
Chloromethane	74-87-3
Dichlorodifluoromethane	75-71-8
Bromomethane	74-83-9
Vinyl chloride	75-01-4
Chloroethane	75-00-3
Methylene chloride	75-09-2
Trichlorofluoromethane	75-69-4
1,1-Dichloroethylene	75-35-4
1,1-Dichloroethane	75-34-3
Trans-1,2-Dichloroethylene	540-59-0
Chloroform	67-66-3
1,2-Dichloroethane	107-06-2
1,1,1-Trichloroethane	71-55-6
Carbon tetrachloride	56-23-5
Bromodichloromethane	75-27-4
Bis(chloromethyl)ether	542-88-1
1,2-Dichloropropane	78-87-5
Benzene	71-43-2
Trans-1,3,-Dichloropropene	542-75-6
Cis-1,3-Dichloropropene	542-75-6
Trichloroethylene	79-01-6
Dibromochloromethane	124-48-1
1,1,2-Trichloroethane	79-00-5
2-Chloroethyl vinyl ether	110-75-8
Bromoform	75-25-2
1,1,2,2-Tetrachloroethene	127-18-4
Toluene	108-88-3
1,1,2,2-Tetrachloroethane	79-34-5
Chlorobenzene	108-90-7
Ethyl Benzene	100-41-4

TABLE A-4. The Eleven Compounds of the Acid Fraction

Compound Name	CAS Registry Number
Phenol	108-95-2
2-Chlorophenol	95-57-8
2-Nitrophenol	88-75-5
2,4-Dimethylphenol	105-67-9
2,4-Dichlorophenol	120-83-2
p-chloro-m-cresol	59-50-7
2,4,6-Trichlorophenol	88-06-2
2,4-Dinitrophenol	51-28-5
4-Nitrophenol	100-02-7
4,6-Dinitro-o-cresol	534-52-1
Pentachlorophenol	87-86-5

APPENDIX B

NOTES TO THE SYSTEM MANAGER

The Gas Chromatography Automation System consists of 22 programs and potentially thousands of files, all in one directory. The system is designed to automatically delete old data. The only attention that the GCAS will need from the system manager will be to add new users and to clean up after analysts who have stopped using the system. These notes provide the information necessary for these functions.

ORGANIZATION OF THE DIRECTORY

The GCAS uses only one directory, namely DZO:GCAS60. This directory must be INITed from the background CLI and never RELEASEd. If DZO:GCAS60 is inadvertently released, and if any user signs off, all of the other users will get UNKNOWN DIRECTORY SPECIFIER errors.

Each user has an account ID of four characters beginning with "GC" and ending with the user's initials. The microcomputer, which the Nova considers to be a user, has the account ID "MIKE". Figure 20 shows how BASIC.ID must be organized for the GCAS.

To protect its integrity, the GCAS is designed to prevent any user from reaching BASIC command level in the directory DZO:GCAS60. When any user logs in, the program MESSAGE.JT is automatically run, as specified in BASIC.ID. MESSAGE.JT must be located in the directory DZO:BASIC, and it must contain the statement CHAIN "INITIALIZE", as shown in Figure 21. In directory DZO:GCAS60, the program named INITIALIZE will chain into the GCAS, as shown in Figure 22, but in other directories, INITIALIZE may be used to start other programs.

An exception to the plan above is necessary to accommodate the microcomputer which transmits data from the Varian to the Nova. Therefore, BASIC.ID specifies a different login message, namely MICROLOGIN.JT, for the account ID MIKE. MICROLOGIN.JT is shown in Figure 23. It must be located in directory DZO:BASIC. There is one other account ID in BASIC.ID which uses MICROLOGIN. This allows the programmer to get into DZO:GCAS60 at BASIC command level for debugging purposes.

FILE NAMES IN THE GCAS

File names in the GCAS adhere to the following conventions:

GCNN	PROGRAM NAME, where NN is the program number.
GCTTTT	METHOD FILE NAME, where TTTT is the method number.
GCOTTTT	TEMPORARY OUTPUT FILE NAME, where TTTT is the method number.
GCOOOOII	ID LIST FILE NAME, where II is the instrument number.
GCTTTTOCC	CONCENTRATION PATTERN FILE NAME, where TTTT is the method number and CC is the position of the concentration pattern letter name in the alphabet.
GCIIMMDDSS	INJECTION DATA FILE NAME, where II is the instrument number, MM is the month, DD is the day, and SS is the sequence number.
GCOOOOOOOO	ARRIVAL FILE NAME.
-.RR	SFC RUN RESULTS FILE NAME.

DELETING UNUSED FILES

If an analyst stops using a particular method or instrument, or stops using the GCAS entirely, many useless files will remain in the system. Deleting such files can easily be done with the background CLI. To get a lineprinter listing of all existing method files and their date of last use, use the CLI command.

```
LIST/A/L/O/S GC****.
```

The name of the person who generated a method can be found by using the method display feature of the GCAS. If you decide to delete a method, you should also delete all of the concentration patterns associated with that method. This can be accomplished by the CLI command

```
DELETE GCTTTT. GCTTTTO**.
```

where TTTT is the method number.

Similarly, to get a lineprinter listing of all existing ID list files, use the CLI command

```
LIST/A/L/O/S GCOOOO**.
```

If you decide to delete an ID list file, you should also delete all of the injection data files associated with that ID list file by using the CLI command

```
DELETE GC0000II. GCII******.
```

where II is the instrument number.

Never release DZO:GCAS60 after using the background CLI.

```
GCTB/DZO:GCAS60/MESSAGE.JT

GCDF/DZO:GCAS60/MESSAGE.JT

GCLM/DZO:GCAS60/MESSAGE.JT

GCDM/DZO:GCAS60/MESSAGE.JT

GCBP/DZO:GCAS60/MESSAGE.JT

GCJK/DZO:GCAS60/MICROLOGIN.JT

MIKE/DZO:GCAS60/MICROLOGIN.JT
```

Figure 20. Required structure of BASIC.ID for the GCAS.

```
0010 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0020 REM   +   LOGIN MESSAGE                                                 +
0030 REM   +   PROGRAM NAME:  MESSAGE.JT                                     +
0040 REM   +   DO NOT DELETE!                                                +
0050 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0060 REM
0078 PRINT
0080 PRINT "     CALL 7314 TO REPORT ANY PROBLEM WITH THE SYSTEM."
0090 REM
0100 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0110 REM   +   THIS SECTION STARTS AUTOMATION SYSTEMS                        +
0120 ON ERR THEN GOTO 0140
0130 CHAIN "INITIALIZE"
0140 ON ERR THEN STOP
0150 REM   +=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+
0160 ESC
0170 NEW
```

Figure 21. Required features of MESSAGE.JT for the GCAS.

```
0010 REM   +=+=+=+
```